Numerical radiative transfer with state-of-the-art iterative methods made easy

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This article presents an on-line tool and its accompanying software resources for the numerical solution of basic radiation transfer out of local thermodynamic equilibrium (LTE). State-of-the-art stationary iterative methods such as Accelerated Λ -Iteration and Gauss-Seidel schemes, using a short characteristics-based formal solver are used. We also comment on typical numerical experiments associated to the basic non-LTE radiation problem. These resources are intended for the largest use and benefit, in support to more classical radiation transfer lectures usually given at the Master level

I. INTRODUCTION

The theory of radiation transfer is of paramount importance for astrophysics. Indeed, except for those objects in the Solar System close enough to us for being explored in situ, from the collection of lunar samples back in the 70's to the spectacular landing of the Philae spacecraft and its instruments on-board, on comet Churyumov–Gerasimenko in November 2014, our knowledge of the Universe overwhelmingly comes from the analysis of the light we collect from distant objects.

For the emblematic case of stars, photons are generated in the central parts of the body. They first scatter across its internal and still opaque layers, finally escaping the star at the bottom of its atmosphere or *photosphere*. These photons will continue to be scattered through the most external layers (and any possible circumstellar structures therein, like for instance solar prominences lying in the corona) of the star, before reaching the interstellar medium and travel into space down to our instruments. Finally, stellar light will scatter again through the Earth atmosphere, when one considers ground-based astronomical observations.

The issue of how radiation transfers along these media of distinct physical nature, in terms of density, temperature, dynamics, magnetic field etc. thus appears as quite obvious. And even though we shall discard hereafter any discussion about terrestrial atmospheric effects, radiation transfer through stellar atmospheres still is a very difficult problem of physics. It relies indeed on complex non-linear light–matter interactions (see e.g., Hubeny & Mihalas 2014^{13}).

The equation of radiative transfer is very likely to be present in all astrophysics courses, more likely at the Master level. Analytical solutions are very few, but they can quite easily be taught and fully derived within a few lectures of introduction to the radiation transfer theory. Despite the often very crude approximations used

in these cases, such solutions may still be very useful to any astronomer willing to "clutch at straws" while facing a problem of interpretation of data (or of numerical results) involving some more or less complicated radiative modelling.

At first glance, the radiative transfer equation (hereafter RTE) appears as a deceptively simple first order ordinary differential equation. This is indeed the case when the so-called source function is already known, and the process of deriving the radiation field from a known source function is referred to as the formal solution. However, in the more general case, the RTE is integro-differential, because the source function depends on integral terms involving the radiation field itself. The general problem of defining self-consistently the radiation field i.e., the specific intensity and its first moments, together with the detailed excitation and ionization states of an atmosphere (and therefore the opacity, as well as the spatial variations of the source function), considering the highly non-linear light-matter interactions which usually take place in astrophysical plasmas is definitely, and still, a (very) difficult problem (see e.g., Rutily & Chevallier 2006^{22}).

A considerable simplification of the problem is brought by the assumption of considering that the astrophysical plasma permeatted by radiation is in the physical conditions of the so-called Local Thermodynamic Equilibrium (hereafter LTE). In such a case, velocity distributions of particles follow a Maxwell–Boltzmann distribution, excitation and ionisation stages of every atom (or molecule) constituting the plasma follow Boltzmann (for excitation equilibrium) and Saha (for ionisation equilibrium) statistics, and the self–consistent source functions are, accordingly, characterized locally by Planck functions (see e.g., Chandrasekhar 1960 10). More insight about the assumptions underlying LTE – and therefore how departures from LTE can take place in a stellar atmosphere – can be found in the monographs of Hubeny & Mihalas (2014) 13

and Oxenius (1986)¹⁹. One should also realize that realistic radiative modelling, even assuming LTE, is such complex already that it actually requires numerical modelling. But even though LTE may be suitable for several astrophysical "objects" (e.g., stellar photospheres), departures from LTE should always be considered as the most general situation. These effects have indeed been identified and studied as early as in the late 60's, with the advent of "numerical radiation transfer" (see e.g., Cuny 1967¹², Mihalas & Auer 1969^{3,4}). However a few analytical solutions to the non–LTE radiation transfer problem may be derived and used for the sake of validating any numerical approach to the problem.

Excluding probabilistic methods such as Monte-Carlo (see e.g., Auer 1968^1 , Bernes 1979^8 and Whitney 2011^{26} for a recent review), we may consider that solutions of the non–LTE radiation transfer equation fall into two main classes being either difference equation methods (e.g., Mihalas & Auer 1969), or $stationary^9$ iterative methods (e.g., Olson, Auer & Buchler 1986 and references therein). Hereafter we shall focus on iterative methods, from the so-called Λ -iteration (or Picard) method to the Jacobi-like approximate or $Accelerated \Lambda$ -Iteration (also known as ALI) method and, finally, the more recent and much less popular still Gauss-Seidel and Successive over-relaxation (SOR) schemes (Trujillo Bueno & Fabiani Bendicho 1995)²⁵.

The treatment of the RTE thus appears to be also a good introduction to numerical techniques, including the use of the moments of a function, in physical sciences.

We first remind basic equations driving the non–LTE (unpolarized) radiation transfer problem in a static and 1D plane-parallel geometry. We shall also restrict ourselves to the special case of monochromatic scattering. Then we shall be able to derive an analytical solution of the NLTE radiation problem. This solution shall therefore be used for testing several iterative methods, including the very popular ALI. Finally, we shall describe a new on-line tool designed for educational purposes. It is located at http://rttools.irap.omp.eu/, and the associated Python software will also be made available from us.

II. FORMAL SOLUTION OF THE RADIATION TRANSFER EQUATION

The derivation of the RTE in a semi-infinite, plane-parallel, static, and 1D geometry can be found in several classic textbooks (Hubeny & Mihalas 2014^{13} , or in the e-book of Rutten 2003^{23}).

The source function is defined as $S_{\nu} = \eta_{\nu}/\chi_{\nu}$ i.e., the ratio bewteen monochromatic emissivity and the extinction or absorption coefficient. The optical depth is defined as $d\tau_{\nu} = -\chi_{\nu}dz$ where $\mu = \cos(\theta)$ and $dz = \mu ds$, assuming that \vec{z} points in the *opposite* direction of gravity and that the direction cosine μ defines the orientation of a ray vs. the z-axis – see Fig. (1). Then RTE comes

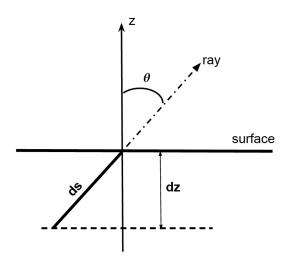


FIG. 1. Geometry of the 1D plane-parallel radiative transfer problem. A ray emerges from a semi-infinite atmosphere with angle θ vs. the normal to the surface \vec{z} . The direction cosine is usually called μ . Along the ray, we use the spatial coordinate s.

into its more familiar form:

$$\mu \frac{dI_{\nu}}{d\tau_{\nu}} = I_{\nu} - S_{\nu} \,. \tag{1}$$

where I_{ν} and τ_{ν} also depend on μ . This basic RTE is the one which appears in most lectures notes and text books introducing radiation transfer to astrophysicists. We shall also assume that the source function is isotropic i.e., angle-independent.

The so-called "formal solution" is the general solution of this equation for a *known* source function. In such as case, the solution can be easily derived as:

$$I_{\nu}(\tau_{1}) = I_{\nu}(\tau_{2})e^{-(\tau_{2}-\tau_{1})/\mu} + \int_{\tau_{1}}^{\tau_{2}} S_{\nu}(\tau_{\nu})e^{-(\tau_{\nu}-\tau_{1})/\mu} \left(d\tau_{\nu}/\mu\right)$$
(2)

We shall see hereafter how this formal solution is used together with iterative methods we are particularly interested in. Note also that, when $\tau_1 \to 0$ and $\tau_2 \to +\infty$ in Eq. (2), the formal solution is the *Laplace* transform of the source function.

A. The Eddington approximation

It is usual and convenient, for analytical radiation transfer, to define the three successive (angular) moments of the specific intensity, or Eddington moments:

$$J_{\nu} = \frac{1}{2} \int_{-1}^{+1} I_{\nu}(\mu) d\mu \tag{3}$$

$$H_{\nu} = \frac{1}{2} \int_{-1}^{+1} I_{\nu}(\mu) \mu d\mu \tag{4}$$

$$K_{\nu} = \frac{1}{2} \int_{-1}^{+1} I_{\nu}(\mu) \mu^{2} d\mu \tag{5}$$

where J is the mean intensity, H the Eddington flux (which relates to the astrophysical flux usually observed for spatially unresolved objects such as most stars other than the Sun), and K which is related to the radiation pressure (see e.g., Hubeny & Mihalas 2014^{13}).

In a similar fashion, successive moments of the RTE can be easily derived. It leads, respectively for Eddington factors H_{ν} and K_{ν} to

$$\frac{dH_{\nu}}{d\tau_{\nu}} = J_{\nu} - S_{\nu} \,, \tag{6}$$

and

$$\frac{dK_{\nu}}{d\tau_{\nu}} = H_{\nu} \,. \tag{7}$$

Then, considering the state of the radiation field at great depth in a stellar atmosphere when it can be safely considered also as isotropic, one can establish the so-called Eddington approximation, $J_{\nu}=3K_{\nu}$ (Rutten 2003²³, Hubeny & Mihalas 2014¹³).

Although valid only in the above-mentioned conditions, it is common in analytical radiation transfer to consider that the Eddington approximation remains valid throughout the whole atmosphere of a star, even though the anisotropy of the radiation field increases while we move towards its most external layers.

B. Λ-operator

It is usual in the field of astrophysical radiation transfer to write the formal solution of RTE as

$$I_{\nu}(\tau) = \Lambda[S(\tau)] \tag{8}$$

where the operator Λ represents the operation of deriving the specific intensity from known opacity and source function spatial distributions. It is also, in other terms, an integration operator of the known source function weighted by the exponential kernel $e^{(t-\tau)}$.

Should we ignore the frequency dependence of the radiation field, also known as the "grey case", and include the angular integration leading from specific intensity to the mean intensity (i.e., a physical quantity proportional to the more generally observed astrophysical flux), one would rather write the formal solution as:

$$J(\tau) = \Lambda[S(\tau)]. \tag{9}$$

For all computations presented hereafter, as well as for the tools we distribute, this process is done using the Python module formal which computes the formal solution using the so-called short characteristics method (Olson & Kunasz 1987¹⁸, Auer & Paletou 1994⁵).

III. AN ANALYTICAL SOLUTION TO A NLTE RADIATION PROBLEM

An analytical solution to the problem of non–LTE radiative transfer can be derived with the following assumptions. First, we shall consider the case of monochromatic or coherent scattering. We shall also consider a source function that contains a thermal emission component εB and a coherent isotropic scattering term $(1 - \varepsilon)J$, that is

$$S = (1 - \varepsilon)J + \varepsilon B. \tag{10}$$

In the frame of the two-level atom model, ε is also called the collisional destruction probability factor (it may also be related to a so-called albedo, with $a = 1 - \varepsilon$ though).

Assuming that the Eddington approximation J=3K is valid at all depths in the atmosphere, we get easily after forming the second derivative of K that

$$\frac{d^2J}{d\tau^2} = 3(J - S). {(11)}$$

For an isothermal atmosphere of constant B with τ and using the expression of the source function introduced at Eq. (10), the latter expression turns into

$$\frac{d^2(J-B)}{d\tau^2} = 3\varepsilon(J-B), \qquad (12)$$

whose solution is such that $(J - B) = \alpha e^{-\tau \sqrt{3\varepsilon}}$.

Finally, using the boudary condition at the surface $J(0) = \sqrt{3}H(0)$ derived by Krook $(1955)^{15}$, one can establish that

$$\alpha = -\frac{B}{1 + \sqrt{\varepsilon}},\tag{13}$$

which leads to the Eddington solution of the non–LTE radiation transfer problem:

$$S_{\text{Edd.}}/B = 1 - (1 - \sqrt{\varepsilon})e^{-\tau\sqrt{3\varepsilon}}$$
. (14)

It is important to identify two critical values associated with this solution. First is the surface value, $S_{\rm Edd.}(\tau)$ for $\tau \to 0$, of the source function given by $\sqrt{\varepsilon}B$. Any

numerical solution have to be tested vs. this limit value, and with some accuracy. Second is the typical depth at which $S_{\rm Edd.} \simeq B$ which is often called the *thermalisation depth*. It scales as $1/\sqrt{\varepsilon}$ for the monochromatic scattering case we consider here. Again this typical length should be identified with accuracy from any numerical solution to the non–LTE problem.

We conclude this section emphasizing the fact that the Eddington solution we have established (for a semi-infinite atmosphere) is the *true* solution of an *approximate* radiation transfer problem. The main approximation used here is on the angular dependence of the specific intensity. While the resolution of the full problem would imply to use an infinite number of directions, we down-sized it to a single point angular quadrature (see also e.g., the discussion provided in §5. of Chevallier et al. 2003).

IV. NUMERICAL SOLUTIONS

We shall consider hereafter monochromatic (or grey) radiation transfer, so we can drop any frequency dependance of the Eddington factors in the remainder of this article. Boundary conditions are also assumed to be monochromatic.

The Eddington approximation is also compatible with the so-called "two-stream approximation". In that case, we adopt also a simplified angular quadrature using $\mu=\pm 1/\sqrt{3}$ (i.e., the Van Vleck angle). Beyond astrophysics, this approximation is also common for global circulation or weather forecasting models developed in (terrestrial) atmospheric sciences (*J.-P. Chaboureau*, private communication). Note again that a proper comparison between numerical solutions and the (analytic) Eddington solution requires the use of a single point angular quadrature.

Our formal solver uses short characteristics (SC) using monotonic parabolic interpolation, as originally described in Auer & Paletou (1994 - see also Olson & Kunasz 1987¹⁸, Kunasz & Auer 1988¹⁴, and Paletou & Léger 2007²¹).⁷. Hereafter we only remind the essential principles of SC, and encourage the reader to consult the existing scientific literature, for details. The numerical implementation of short-characteristics rely on the following principles. Short characteristics means that the formal solution across the whole atmosphere will be carried-out depth after depth, from one boundary surface to the other one, and back-and-forth i.e., for μ negative first then for μ positive (note that this order is indifferent, but the separation between positive and negative direction cosines is very important, and shall prove very useful for the case of Gauss-Seidel iterations). In order to perform at each spatial depth the formal solution expressed by Eq. (2), we shall first assume that the source function is quadratic in the optical depth. This assumption allows to derive an analytical expression of the integral term on the source function spatial distribution. Then it can easily be shown that, for a current position k the integral in Eq. (2) will

only involve quantities known at this very position, and at the "upwind" or (k-1), and "downwind" or (k+1) positions. Finally, at each depth the current value of the specific intensity (for a given direction cosine) will be given by

$$I_k = I_{k-1}e^{-\Delta\tau_u} + \Psi_u S_u + \Psi_0 S_0 + \Psi_d S_d, \qquad (15)$$

where the Ψ 's are analytical functions of the optical depths $\Delta \tau_u$ and $\Delta \tau_d$ i.e., between the local (0), and the upwind (u) and downwind (d) spatial positions.

For all cases discussed hereafter, we use boundary conditions more usually used for "semi-infinite" atmospheres. There is no radiation falling ($\mu < 0$) onto the top surface of the atmosphere, and the bottom and upward ($\mu > 0$) boundary condition is that the specific intensity equals the Planck function (set to one hereafter).

A. Λ -iteration

The so-called Λ -iteration (LI) is equivalent to a Picard iterative scheme (itself being a fixed-point iterative scheme for ODEs).

Let S^{\dagger} be the spatial distribution of the source function across the atmosphere from (the initial value or) the previous iteration step. Λ -iterating consists in successively computing

$$J = \Lambda[S^{\dagger}], \tag{16}$$

then $S^{(\text{new})} = (1-\varepsilon)J + \varepsilon B$ and so on, until convergence. Unfortunately, this poor numerical scheme is still in use although it is well-known that it is "pseudoconvergent" (see e.g., Hubeny & Mihalas 2014¹³, Olson et al. 1986¹⁷). This is well demonstated by Figs. (2) where we displayed (a) the successive iterates of the LI scheme together with the target analytical solution of Eddington and, (b) the respective relative correction, from an iteration to another, R_e and the so-called "true error" T_e , which is the relative error vs. the analytical Eddington solution.

Following the definitions found in the original papers of Auer et al. (1994)⁶ and Trujillo Bueno & Fabiani Bendicho (1995)²⁵, these two latter quantities are respectively

$$R_e = \max(|S^{(n)} - S^{(n-1)}|/S^{(n)}) \tag{17}$$

$$T_e = \max(|S^{(n)} - S_{\text{Edd.}}|/S_{\text{Edd.}}).$$
 (18)

Both are indeed useful to demonstrate the pseudo-convergent nature and the *failure* of LI. Indeed on Fig. (2b) once can notice the constant drop of the relative correction R_e giving the misleading impression that pushing the iteration number will finally reach the solution, while the true error T_e indicates that the pseudo-solution will remain far away from the reference solution of Eddington.

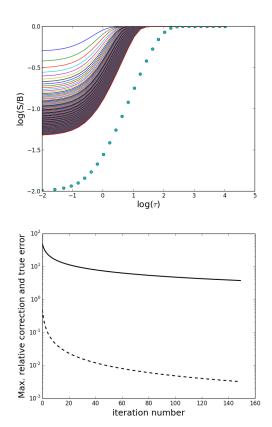


FIG. 2. Λ -iteration for a semi-infinite slab of total optical thickness 10^4 with 5 points per decade, and an atmosphere such as $\varepsilon = 10^{-4}$. The top figure shows the successive runs of the source function, and the pseudo-convergent nature of the numerical scheme. The analytical solution is represented by the dotted curve. The bottom figure displays (i) the maximum relative correction, from an iteration to another (dashed line), and (ii) the true error i.e., the relative error vs. the analytical solution (note that we always have $T_e > R_e$ after a few iterations).

Note also that, in all figures $T_e > R_e$ after the very first iterative steps, if not at the onset of the iterative process.

B. ALI: Accelerated/Approximate Λ -iteration

The ALI method is basically an operator splitting method. Let us write therefore:

$$\Lambda = \Lambda^* + \delta \Lambda \,. \tag{19}$$

At this point several choices for an approximate operator Λ^* are possible. However, in our study we shall only consider the most efficient version of ALI which is just a Jacobi-type method. In such a case, Λ^* should be the exact diagonal of the full operator Λ . The study of reference concerning this very method is the seminal article

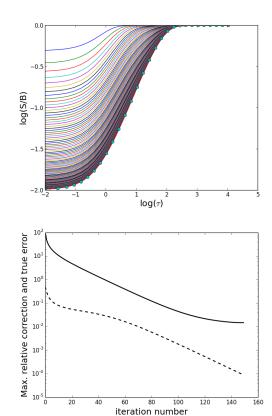


FIG. 3. Same as Fig. (2) but for Accelerated Λ -iteration. Within the same number of iterations (150) the analytical reference solution is reached, unlike with LI. The true error reaches a constant level around 0.01, also indicating that there is no need to iterate further than ~ 140 iterations, while the relative correction continues to decrease.

of Olson, Auer & Buchler $(1986)^{17}$. In practice, the diagonal operator is very easily determined, as described in Auer & Paletou $(1994)^5$

Now let us write the succession of iterates of the source function as $S = S^{\dagger} + \delta S$, where S^{\dagger} means the source function known at the current iterative step. Now using the definition of the Λ -operator $J = \Lambda[S]$ we can write the expression of the source function correction explicitely:

$$\delta S = \left[1 - (1 - \varepsilon)\Lambda^*\right]^{-1} \left\{ (1 - \varepsilon)\Lambda[S^{\dagger}] + \varepsilon B - S^{\dagger} \right\}. \tag{20}$$

When Λ^* is the diagonal of the full operator, at each depth in the atmosphere the increment of source function is just obtained from a *scalar* divide, which make the ALI method both accurate and fast.

Unlike the LI iteration, it can be rigorously shown that the ALI iterative scheme definitely converges to the solution of the problem, as demonstrated in Fig. (3a). However, the accuracy of the numerical solution depends on the spatial sampling of the atmosphere. It can be measured by the true error, T_e , which reaches a plateau at $\sim 10^{-2}$, as can be seen in Fig. (3b).

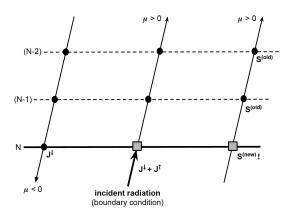


FIG. 4. Illustration in support of the basic principle of the implementation of Gauss–Seidel iterations within the short characteristics method.

C. Gauss-Seidel and SOR iterations

Experimenting both Gauss–Seidel (GS) and Successive over-relaxation (SOR) are logical steps after having experienced the Jacobi-type ALI methods. Although published twenty years ago now, by Trujillo Bueno & Fabiani Bendicho $(1995)^{25}$, it is not yet of common practice, unlike ALI.

The GS iterative method consists essentially in updating the current source function value once the full angular integration of the specific intensity can be performed - because all the necessary quantities yet are available, and before the formal solver will be moving to the next depth point. This is made relatively easy within the short characteristics methods which separates sweping the atmosphere first for $\mu < 0$ and second for the remainder $\mu > 0$ directions (or vice versa, the important point being an explicit distinction between positive and negative direction cosines). This is sketched in Fig. (4) which should be read from left to right. Assume that all depths have been covered along SC's of $\mu < 0$, so that we know all specific intensities and mean intensities J^{\downarrow} for these direction cosines, up to the bottom boundary layer N. The next task is to complete the angular integration for the upward direction cosine(s). Starting at the bottom boundary, the "upwind" specific intensity is known since it is provided by the external boundary condition. Therefore, at layer N we can easily compute J^{\uparrow} . This knowledge makes it possible to update the local source function before switching to the next inner layer at (N-1). This is the main "trick" for doing Gauss-Seidel iterations within the SC method. It requires however modifications of the more traditional formal solver used for ALI (provided by us as the formalGS module). Indeed, when moving to the next layer for $\mu > 0$ at (N-1), we shall advance the specific intensity according to Eq. (15) but now using a mixture of the just updated $S_u^{\text{(new)}}$ and of $S_{0,d}^{\text{(old)}}$ i.e., of the not yet modified values of the source function at the local and at the downwind position (N-2). The process

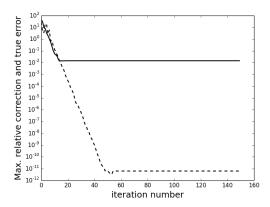


FIG. 5. True error and relative correction (dashed line) for the same parameters than in previous figures, but using the GS iterative scheme. The truncation error seen by the *plateau* at $T_e \sim 10^{-2}$ is reached in less than 30 iterations now.

is then repeated up to the top boundary surface of the atmosphere.

The numerical implementation of the method was described in every detail in the original article of Trujillo Bueno & Fabiani Bendicho (1995)²⁵. We therefore strongly encourage the reader to study this article with great care.

Figure (5) shows the significative gain on the convergence rate provided by GS. For 1D problems, it is by far superior to the small additional computations induced by the indispensable modifications of the classical short characteristics formal solver.

Finally the SOR scheme is built on the same strategy adopted for GS although the new source function increment $\delta S^{({\rm SOR})} = \omega \delta S^{({\rm GS})}$, with ω chosen between 1 and 2. It can be shown that the optimal scheme is obtained for $\omega \sim 1.5$ (see Trujillo Bueno & Fabiani Bendicho 1995²⁵) More insight about the SOR method can be found in Young (1971).²⁷

V. NLTE RADIATION TRANSFER ON-LINE

We have implemented a dedicated web-service which allows on-line numerical experiments with the numerical methods we just presented. It is located at http://rttools.irap.omp.eu/, and maintained by OMP-IRAP (Toulouse, France). In addition, a Git repository is about to be installed, in order to distribute the original Python modules we developed and used for the web-service.

A. Description

Several "buttons" may be independently activated. The first choice is to be made among methods i.e., Λ -iteration (LI), Accelerated Λ -iteration (ALI), and Gauss-

Seidel or SOR (GS). Concerning the latter choice, the distinction between both schemes will be controled by the ω (omega) parameter. Once the method have be selected, the user will have to provide a value for ε (eps) with format 10^{-p} where p is an integer, the total optical thickness of the atmosphere $\tau_{\rm max}$ (taumax), using a format 10^k , and the number of points per decade (npdec) used for setting the spatial grid for the computations. Finally, the number of iterations (niter) to be performed is required.

The output consists in two graphics. The first one provides the history of the source function (initialized with $S \equiv B$) for the number of iterations required, with the corresponding Eddington solution vs. optical depth. The second plot displays both true error and relative correction (from an iteration to another) vs. the number of iterations.

B. Experiments

As a preamble to this part, we remind here that comparison with the analytical solution of Eddington make only sense for the case of "effectively thick" slabs, that is such that $\tau_{max} \gg 1/\sqrt{\varepsilon}$, for the case of monochromatic scattering we only consider hereafter.

A first and *indispensable* experiment is to realize the failure of the Λ -iteration. The "pseudo-convergence" of this method can be noticed by the rapid and continuous fall of the relative correction R_e , while the "solution" at which the process is converging may remain very far from the Eddington solution, as indicated by the "true" error T_e . Further experiments pushing the number of iterations for the same set-up should be done and analysed.

Using the very same set of parameters, the next step is to experiment the benefit of the diagonal operator ALI method. The latter should quickly reach the Eddington solution with good accuracy, unlike LI. Other experiments will allow to check the so-called $\sqrt{\varepsilon}$ -law for the surface value of S/B, as well as to identify the "thermalisation depth" $1/\sqrt{\varepsilon}$.

However, even ALI may work at limited accuracy. A relevant experiment is to iterate the method with a given set of parameters up to reaching a plateau for T_e . The latter value gives an indication of the truncation error of the method, due to the spatial discretization of the numerical method. All other parameters remaining equals, one should then experiment the effects of only modifying the sampling of the slab, by changing the number of points per decade parameter. Changes in the limit value of T_e , together with the rate of convergence should be investigated. Note that a detailed study on the accuracy of the ALI method was published by Chevallier et al. (2003).

Finally, we propose to go beyond the ALI–Jacobi method with the Gauss–Seidel (GS) and Successive Over-Relaxation (SOR). Its implementation requires several touchy modifications in the original short characteristics formal solver which require special attention. We found them pretty well documented in the original article, and the interested user will get to it by a careful inspection of the source code that we also deliver with our webservice. Gauss-Seidel and SOR differ only by the choice of the relaxation parameter ω . It should be set to $\omega=1$ for performing GS iterations, although it should be picked between 1 and 2 for experimenting SOR iterations. It is a good exercice to test various values of ω , seeking for an optimal scheme.

A more insider study, requiring to use directly the Python code we make available, would be to test the so-called smoothing capability of GS/SOR methods which plays a crucial role in multi-grid methods (see e.g., Auer et al. 1994^6)

VI. CONCLUSION

We made available a tool very suitable to any astrophysics Master programme, or for any astronomer or physicist willing to start an initiation to state-of-the-art numerical radiation transfer.

It is quite straightforward to upgrade the simple angular quadrature we used for that study. It would be also possible to implement, from our Python formal solver, the computation of a more realistic scattering integral, by integrating an explicitly ν -dependent mean intensity J_{ν} weighted by an a priori known absorption profile (Gaussian/Doppler or Voigt).

Possible evolutions may be, to develop a specific formal solver for the 1D spherical problem (see e.g., Auer 1984^2), or to propose a *simple* multi-level atom version following the so-called Multilevel-ALI method originally developed by Rybicky & Hummer (1991, see also Paletou & Léger 2007). Comparisons with (non-stationary) conjugate gradient type method could also be set-up (see e.g., Paletou & Anterrieu 2009^{20}).

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